Nonadiabatic dynamics of a Bose-Einstein condensate in an optical lattice

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We study the nonequilibrium dynamics of a Bose-Einstein condensate that is split in a harmonic trap by turning up a periodic optical lattice potential. We evaluate the dynamical evolution of the phase coherence along the lattice and the number fluctuations in individual lattice sites within the stochastic truncated Wigner approximation when several atoms occupy each site. We show that the saturation of the number squeezing at high lattice strengths, which was observed in recent experiments by Orzel *et. al.*, can be explained by the nonadiabaticity of the splitting.

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Ultra-cold atomic gases in periodic optical lattice potentials have recently attracted considerable interest and inspired experiments, e.g., on the Bose-Einstein condensate (BEC) coherence [1, 2], superfluid dynamics [3, 4, 5], the number-squeezed [6] and the Mott insulator (MI) [7] states, and quantum information applications [8, 9]. An optical lattice provides a clean many-particle system with enhanced interactions, resulting in a unique opportunity to study strong quantum fluctuations. While the classical mean-field theories, such as the Gross-Pitaevskii equation (GPE), have been successful in describing the full multi-mode dynamics of weakly-interacting BECs, they have severe limitations in optical lattices, as they disregard thermal and quantum fluctuations, decoherence, and the information about quantum statistics. In this paper we study matter wave dynamics beyond the GPE by considering a harmonically trapped finite-temperature BEC that is dynamically split by an optical lattice potential. We show that the experimentally observed saturation of the number squeezing at high lattice strengths [6] can be explained by the nonadiabaticity of the loading of atoms into the lattice. The thermal and quantum fluctuations are included within the truncated Wigner approximation (TWA). The multi-mode TWA provides a natural representation for the dynamical fragmentation of the initially uniform BEC in the lattice and the transition to the regime that can also be described by the discrete Bose-Hubbard Hamiltonian (BHH). Moreover, the resulting highly occupied number squeezed states are also of great interest in the Heisenberg limited interferometry [6, 10].

We study the loading of atoms into the lattice within the TWA. The TWA may be obtained by using the familiar techniques of quantum optics [11, 12] to derive a generalized Fokker-Planck equation (FPE) for the Wigner distribution of the trapped multi-mode BEC [13]. The TWA consists of neglecting the dynamical quantum noise, acting via third-order derivatives in the FPE, and results in a deterministic equation for the classical field ψ_W which coincides with the GPE:

$$i\partial_t \psi_W = \mathcal{L}\psi_W + g|\psi_W|^2\psi_W \,, \tag{1}$$

where $\mathcal{L} \equiv -\hbar^2\nabla^2/(2m) + V$. The thermal and quantum fluctuations are included in the initial state of ψ_W in Eq. (1) which represents an ensemble of Wigner distributed wave functions. The neglected terms are small when the amplitudes of the Wigner distribution are large. The TWA and closely related approaches have previously been successful in describing atomic BECs [13, 14, 15, 16, 17, 18] and optical squeezing [19]. In particular, the TWA is shown to produce correctly, e.g., the Beliaev-Landau damping [15] and it has been argued that the TWA more generally provides an accurate description for the short-time asymptotic behavior of the full quantum dynamics [17].

We consider a BEC in a tight elongated cigar-shaped trap, with the trap frequencies $\omega \equiv \omega_x \ll \omega_{y,z} \equiv \omega_\perp$, and ignore the density fluctuations along the transverse directions. This results in an effective 1D GPE for $\psi_W(x,t)$ with $g = g_{1D} = 2\hbar\omega_\perp a$ in Eq. (1), where a denotes the scattering length. The BEC is initially assumed to be in thermal equilibrium in a harmonic trap $V_h(x) = m\omega^2x^2/2$. A self-consistent calculation of the initial state would involve solving the coupled Hartree-Fock-Bogoliubov equations for the condensate and non-condensate populations [20]. Here we resort to a simpler Bogoliubov approximation and expand the field operator $\hat\psi(x,t=0)$ in terms of the BEC ground state amplitude $\hat\alpha_0\psi_0$, with $\langle\hat\alpha_0^\dagger\hat\alpha_0\rangle = N_0$, and the excited states:

$$\hat\psi(x) = \psi_0(x)\hat\alpha_0 + \sum_{j>0}\left[u_j(x)\hat\alpha_j - v_j^*(x)\hat\alpha_j^\dagger\right], \tag{2}$$

where $u_j(x)$ and $v_j(x)$ ($j>0$) are obtained from

$$\begin{aligned}\left(\mathcal{L}-\mu+2N_0g_{1D}|\psi_0|^2\right)u_j - N_0g_{1D}\psi_0^2 v_j &= \epsilon_j u_j\,,\\ \left(\mathcal{L}-\mu+2N_0g_{1D}|\psi_0|^2\right)v_j - N_0g_{1D}\psi_0^{*2} u_j &= -\epsilon_j v_j\,.\end{aligned} \tag{3}$$

Here $\hat\alpha_j$ are the quasiparticle annihilation operators, with $\langle\hat\alpha_j^\dagger\hat\alpha_j\rangle = \bar n_j \equiv [\exp(\beta\epsilon_j)-1]^{-1}$, $\beta \equiv 1/k_BT$, and ψ_0 is ground state solution of the GPE with the chemical potential μ.

In the Wigner description we replace the quantum operators $(\hat{\alpha}_j, \hat{\alpha}_j^\dagger)$ (for $j>0$) by the complex random variables (α_j, α_j^*), obtained by sampling the corresponding Wigner distribution of ideal harmonic oscillators in a thermal bath [11]:

$$W(\alpha_j, \alpha_j^*) = \frac{2}{\pi}\tanh(\xi_j)\exp\left[-2|\alpha_j|^2\tanh(\xi_j)\right], \quad (4)$$

where $\xi_j \equiv \beta\epsilon_j/2$. The Wigner function is Gaussian distributed with the width $\bar{n}_j + \frac{1}{2}$. The nonvanishing contribution to the width at $T=0$ for each mode represents the quantum noise. The Wigner function returns symmetrically ordered expectation values, so $\langle\alpha_j^*\alpha_j\rangle_W = \bar{n}_j + \frac{1}{2}$, and $\langle\alpha_j\rangle_W = \langle\alpha_j^*\rangle_W = \langle\alpha_j^2\rangle_W = 0$, etc.

For large BECs, $N_0 \gg 1$, the main contribution to the matter wave coherence in the superfluid regime is due to the thermal and quantum fluctuations of low-energy phonons and the quantum fluctuations of the initial harmonically trapped BEC mode are not very important. Consequently, we could treat the BEC mode $\hat{\alpha}_0$ even classically. However, here we assume it to be in a coherent state and sample the quantum fluctuations according to the corresponding Wigner distribution [11]: $W(\alpha_0, \alpha_0^*) = 2\exp(-2|\alpha_0 - N_0^{1/2}|^2)/\pi$, so that $\langle\alpha_0\rangle_W = N_0^{1/2}$ and $\langle\alpha_0^*\alpha_0\rangle_W = N_0 + \frac{1}{2}$. Since we compare the matter wave coherence between the atoms in different lattice sites, the global BEC phase is unimportant. The advantage of using the coherent state description is that the Wigner function is positive.

Due to the symmetric ordering of the expectation values obtained from the Wigner distribution, it is difficult, or even impossible, to extract several correlation functions for the full multi-mode field operator, since the Wigner field is symmetrically ordered with respect to *every* mode. In [13] the phase diffusion of a BEC was therefore calculated by defining a 'condensate mode' operator associated with the projection of the stochastic field onto the ground state solution. Since we study the splitting of a BEC by a periodic optical lattice potential, it is useful to define analogously the ground state operators a_j for each individual lattice site j:

$$a_j(t) = \int_{j^{\rm th}\,\rm well} dx\, \psi_0^*(x,t)\psi_W(x,t), \quad (5)$$

where $\psi_W(x,t)$ is the stochastic field, determined by Eq. (1), and $\psi_0(x,t)$ is the ground state wave function at time t, obtained by integrating the GPE in imaginary time in the potential $V(x,t)$. The integration is over one lattice site. For each lattice site ground state mode a_j, the normally ordered expectation values can be easily obtained $\langle a_i^* a_j\rangle_W = \langle\hat{a}_i^\dagger\hat{a}_j\rangle + \delta_{i,j}/2$, etc.

The BEC is initially assumed to be in a harmonic trap and we continuously increase the strength of the optical lattice potential until some final value, after which the potential is kept constant, $V(x,t) = V_h(x) + s(t)E_r\sin^2(\pi x/d)$, with $s(t) = \exp(\kappa t) - 1$ for $t \le \tau$ and $E_r = \hbar^2\pi^2/(2md^2)$, where $d = \lambda/2\sin(\theta/2)$ is the lattice period, obtained by two laser beams intersecting at an angle θ. For very large s and close to the ground state only one mode per lattice site is important and the system can be approximated by the BHH:

$$H = \sum_i \left[\nu_i\hat{b}_i^\dagger\hat{b}_i - J(\hat{b}_i^\dagger\hat{b}_{i+1} + \text{H.c.}) + \frac{U}{2}(\hat{b}_i^\dagger)^2\hat{b}_i^2\right], \quad (6)$$

where the summation is over the lattice sites, $J \simeq -\int dx\eta_i^*(x)\mathcal{L}\eta_{i+1}(x)$ is the hopping amplitude between the nearest-neighbor sites, $U \simeq g_{1D}\int dx|\eta_j(x)|^4$, and $\nu_j \equiv j^2d^2m\omega^2/2$, with $j=0$ site at the trap center. We may approximate the Wannier functions η_i by the ground state harmonic oscillator wave function with the frequency $\omega_s = 2s^{1/2}E_r/\hbar$ at the lattice site minimum [21]. When we compare the TWA results to the BHH, we frequently extract the expectation values involving $\hat{b}$ using Eq. (5) with $\hat{b} \sim \hat{a}$. We tested that using different projections does not affect the results. For $n_iJ \gtrsim U$, with $n_i \equiv \langle\hat{b}_i^\dagger\hat{b}_i\rangle$, the system is in the superfluid regime with the long-range phase coherence and is expected to undergo the MI transition at $n_iJ \sim U$ [22], resulting in a highly number squeezed ground state.

In the numerical studies of loading the BEC into an optical lattice, we first solve the BEC ground state ψ_0 by evolving the GPE in imaginary time in the harmonic trap and then diagonalize Eq. (3) to obtain the quasiparticle mode functions u_j, v_j and energies ϵ_j. The time evolution of the ensemble of Wigner distributed wavefunctions [Eq. (1)] is unraveled into stochastic trajectories, where the initial state of each realization for ψ_W is generated according to Eq. (2) with the operators replaced by the Gaussian-distributed random variables (α_j, α_j^*). We integrate Eq. (1) using the split-step method and in several cases the sufficient convergence is obtained after 600 realizations. The convergence is generally slower at higher temperatures. Unlike the 3D TWA [15], the 1D simulations do not similarly depend on the total number of quasiparticle modes and we found the calculated results to be unchanged when we increased the number of modes.

For the typical nonlinearity $N_0g_{1D} = 100\hbar\omega l$, with $l \equiv (\hbar/m\omega)^{1/2}$, the initial harmonically trapped BEC is well described by the GPE with the Poisson density fluctuations and the ratio between the interaction and the kinetic energy $\gamma = mg_{1D}/(\hbar^2 n_{1D}) \lesssim 10^{-3}$ [23], where n_{1D} is the 1D atom density. The corresponding initial Thomas-Fermi radius $R/l = (3N_0g_{1D}/2\hbar\omega l)^{1/3} \simeq 5.3$. We take $d = \pi l/8$, resulting in $E_r = 32\hbar\omega$. Within $2R$, we then have 30-35 lattice sites. A similar number of sites has also been realized in recent experiments in a cigar-shaped trap with $d \simeq 2.7\mu$m [2]. In order to characterize the phase coherence along the lattice, we introduce the normalized first-order correlation function between the central well and its ith neighbor as $C_i \equiv |\langle\hat{a}_0^\dagger\hat{a}_i\rangle|/\sqrt{n_0n_i}$.

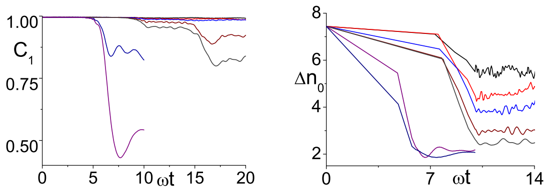

FIG. 1: The phase coherence between the central well and its nearest neighbor C_1 as a function of time (left) at $T = 0$ for different final heights of the optical lattice (curves from top represent $s = 5, 8, 10, 15, 20, 30, 40$ with the atom number in the central well $n_0 \simeq$90-100). The ramping time $\omega\tau = 10$, except for $s = 30, 40$, $\omega\tau = 6$. The number fluctuations Δn_0 for the central well (right) for the same runs. Here $g_{1D} = 0.05\hbar\omega l$ and $N_0 = 2000$. The number squeezing can be accurately fitted according to $(\Delta n_0)^2/n_0 \simeq 0.03+0.5e^{-s/8} \simeq 0.03+0.3J^{0.4}$.

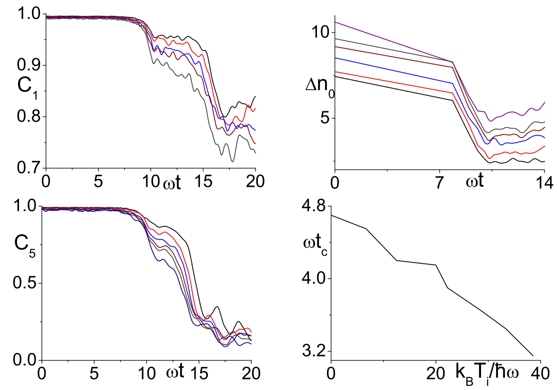

FIG. 2: The coherences C_1 (top left), C_5 (bottom left) and the number fluctuations Δn_0 (top right) for initial temperatures (curves from top) $k_B T_i/\hbar\omega = 0, 12.5, 22.2, 33.3, 38.5$ (C_5 also with 28.5). The phase collapse time t_c (bottom right) is evaluated at $C_5 = 0.5$. The same system as Fig. 1 with $s = 20$.

In Fig. 1 we show C_1 and the number fluctuations $\Delta n_i = [\langle(\hat{a}_i^\dagger \hat{a}_i)^2\rangle - \langle\hat{a}_i^\dagger \hat{a}_i\rangle^2]^{1/2}$ in the central well for different final heights of the periodic potential at $T = 0$. For shallow lattices the phase coherence remains high and steady, but for larger s it is reduced and becomes strongly oscillatory. Due to the large occupation numbers, Δn_0 are strongly sub-Poissonian, approaching the asymptotic value $(\Delta n_0)^2/n_0 \simeq 0.03 \ll 1$ for large s. Here the MI transition for the ground state is expected to occur at $s \simeq 30$. However, we find $\Delta n_0 \gtrsim 1$ for all s, which can be understood by the nonadiabatic loading.

For an adiabatic turning up of the lattice and for the system to remain in its ground state, we require that the rate of change in the tunneling amplitude to be slower than any characteristic time scale of the system. At low lattice heights it is more difficult to avoid exciting higher vibrational levels within one potential well, resulting in excitations in the higher energy bands. Moreover, the phonon mode energies ω_n in the lowest energy band decrease with increasing lattice strength [24, 25] and for high lattices it is more difficult to maintain the adiabaticity with respect to these excitations. In Fig. 1 we find the number squeezing to saturate around s=20-30, indicating the point when an increasing number of phonon modes is excited and the loading becomes strongly nonadiabatic. Consequently, the $s \geq 15$ cases exhibit significant excess number fluctuations as compared to the ground state. After a short time period over which C_1 remains constant, the large Δn_i evolve into large phase fluctuations and C_1 becomes oscillatory and collapses.

The saturation of the number squeezing for strong lattices was experimentally observed in [6] for a 3D vapor in a 1D lattice. Such a system is not tightly elongated, but we can still make qualitative comparisons to the experimental data. Although the saturation was assumed in [6] to be an artifact of the analysis method of the interference measurement, we also numerically find the same saturation effect which can be explained by the nonadiabaticity of the loading process. If the loading is sufficiently rapid or the final lattice sufficiently high, so that the adiabaticity breaks down for a large number of modes, the optimal number squeezing is proportional to the ramping speed itself and the nonlinearity. Both in Fig. 1 and in [6] the squeezing saturates at about 15dB when $n_i U/J \sim 10^4$. The ramping time $\tau \simeq 4000\hbar/E_r$ in [6] is one order of magnitude longer than in Fig. 1, but this is compensated by the weaker hopping amplitude J, so that the saturation roughly occurs at the same value of $\omega_n\tau$.

Although the BHH (6) is only valid for weakly excited high lattices, it is interesting to compare the TWA results to the Bogoliubov approximation to the BHH. These were calculated in the homogeneous lattice ($\nu_i = 0$) in [24, 25, 26]. Similarly, we may diagonalize the linearized fluctuations in Eq. (6) around the ground state atom density with the fluctuation part $\delta\hat{b}_j = \sum_n [f_n(jd)\hat{\chi}_n - h_n^*(jd)\hat{\chi}_n^\dagger]$, resulting in the number fluctuations in each site, $(\Delta n_i)^2 = n_i \sum_j |w_j|^2(2\bar{n}_j+1)$, and the phase fluctuations between the k and l sites, $(\Delta\varphi_{kl})^2 \equiv \langle(\hat{\varphi}_k - \hat{\varphi}_l)^2\rangle = 1/4\sum_j |r_j(kd)/\sqrt{n_k} - r_j(ld)/\sqrt{n_l}|^2(2\bar{n}_j+1)$, where $\hat{n}_i = \sqrt{n_i}\sum_j(w_j\hat{\chi}_j + w_j^*\hat{\chi}_j^\dagger)$ and $\hat{\varphi}_i = -i/(2\sqrt{n_i})\sum_j(r_j\hat{\chi}_j - r_j^*\hat{\chi}_j^\dagger)$ are the number and phase operators, with $w_j \equiv f_j - h_j$, $r_j \equiv f_j + h_j$, and $\bar{n}_j = \langle\hat{\chi}_j^\dagger\hat{\chi}_j\rangle$. In the homogeneous lattice with n atoms per site we have $(\hbar\omega_q)^2 = 4J\sin^2(qd/2)[4J\sin^2(qd/2)+2nU]$, where q is the quasiparticle momentum [24, 25]. Moreover, for $nU \gg J$ and N_p lattice sites, $(\Delta n_i)^2 \simeq \sum_q \hbar\omega_q/(2UN_p)(2\bar{n}_q+1)$ and $(\Delta\varphi_{k,k+1})^2 \simeq \sum_q \hbar\omega_q/(4nJN_p)(2\bar{n}_q+1)$, which at $T=0$ approximately yield $(8nJ/U)^{1/2}/\pi$ and $(2U/nJ)^{1/2}/\pi$, respectively. Numerically, we find the Bogoliubov results in the harmonic trap for Δn_0 to be slightly larger and for $\Delta\varphi_{01}$ smaller than the homogeneous result. The TWA results for Δn_i in Fig. 1 are clearly larger than the ideal Bogoliubov limit, however, $(\Delta n_0)^2/n_0 \propto J^{0.4}$ still qualitatively similar to the Bogoliubov result (n_0U depends

only weakly on s). As argued in [24], if the adiabaticity of a phonon mode breaks down, the number fluctuations of the mode freeze to the value that prevails at the time this occurs, i.e., when $\omega_j \sim \zeta(t) \equiv |\partial_t J(t)/J(t)|$. Using the homogeneous lattice result at $T = 0$ we obtain $(\Delta n_i)^2 \simeq \sum_j \hbar\zeta_j(t_j)/(2UN_p)$. Since for all j, $\zeta_j(t_j)$ is here roughly of the order of ω, we have the asymptotic value for $s \to \infty$, $(\Delta n_i)^2 \sim \hbar\omega/U$, qualitatively similar to Fig. 1. In order to study the effect of the nonlinearity we also varied in the simulations $N_0 g_{1D}/\hbar\omega l$ from 100 to 400 for $s = 20$ and found $(\Delta n_0)^2/\sqrt{n_0} \propto U^c$, with $c \simeq -0.26$, as compared to the Bogoliubov result $c = -1/2$.

In Fig. 2 we show Δn_0 and the coherence C_1 for different initial temperatures T_i for $s(\tau) = 20$. Here $(\Delta n_0)^2$ increases exponentially as a function of T_i. The phase coherence C_5 between the central well and its 5th neighbor decays significantly faster than C_1. The dependence of the phase collapse time t_c on T_i is approximately linear. At $s = 20$ the effects of the harmonic trap are already significant, since the variation of the trapping potential over five sites exceeds the tunneling energy $\nu_5 \simeq 2\hbar\omega \gtrsim n_0 J$.

If the lattice potential is turned up adiabatically, the population of each mode remains constant and temperature T can change dramatically, as the contribution of each mode to T changes by the ratio of the final and initial mode energies $\omega_j^{(f)}/\omega_j^{(i)}$. An adiabatic increase in the lattice strength may both increase or lower T, depending on whether the excited band is occupied [27] and in the experiments the condensation temperature has been found to be sensitive to the lattice height [28]. In Fig. 3 we estimated the population and the 'temperature' of the lowest phonon modes in the TWA simulations by evaluating the projection of ψ_W to the Bogoliubov modes of the BHH (6). The averages are taken over a time period before any significant rethermalization occurs after the ramping. The modes 2 and 4 are highly excited for the case of short τ, due to the nonadiabatic loading. The excitations are damped out at higher T_i and for $\omega\tau = 30$, corresponding to $\omega_{2,4}\tau \gg 1$. It is interesting to note that the excitations of the forth mode are only damped out when the rate of change in the tunneling amplitude ζ is much smaller than the corresponding mode energy, or when $\omega_4 \simeq 26\zeta(\tau)$. This is more restrictive condition than the one found in [24]. For $\omega\tau \lesssim 3$, the variation of T_i is already completely dominated by the excitations due to the rapid turning up of the lattice.

The advantage of 1D lattices is that the lattice spacing can be easily modified by using non-parallel lasers. A large spacing could even allow the scattering of light, or the Bragg spectroscopy, from individual lattice sites and the separate optical detection of number fluctuations in each site, using a similar analysis to [29]. Moreover, an interference measurement on the expanding atoms can provide detailed information about the coherence [2].

We studied the loading of a harmonically trapped BEC into an optical lattice. In a good agreement with experiments [6], we found the number squeezing to saturate for high lattices, which can be explained by the finite ramping time of the lattice potential. It is numerically more demanding to study a truly adiabatic loading for strong lattices. However, it would be particularly interesting to examine the validity of the TWA close to the MI ground state. Our analysis seems to indicate that, in the case of lattices with large filling factors, the ramping time required to reach the MI state may be very long and can be demanding in actual experiments. In the lattice experiments the atoms are also coupled to environment, resulting in dissipation with the system relaxing towards its ground state. We could improve our model, e.g., by incorporating the spontaneous emission due to the lattice lasers. This would introduce also a dynamical noise term in Eq. (1). However, experimentally spontaneous emission can also be avoided since, e.g., with intense CO_2 lasers the spontaneous emission rate is very low [30]. Finally, our TWA studies could also be extended to the finite temperature damping of nonequilibrium oscillations in a multi-well BEC what has previously been studied in double-well BECs [31].

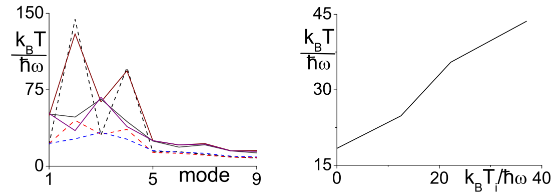

FIG. 3: The contribution of the lowest modes to temperature (left) for $k_B T_i/\hbar\omega = 12.5$ (dashed line) and 37 (solid line). The curves from top $\omega\tau = 10, 20, 30$ for both cases. The average temperature of the first five modes after the ramping $\omega\tau = 30$ (right). Here $g_{1D} = 0.015\hbar\omega l$, $N_0 = 2000$, and $s = 5$.

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